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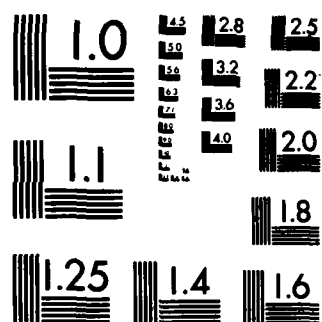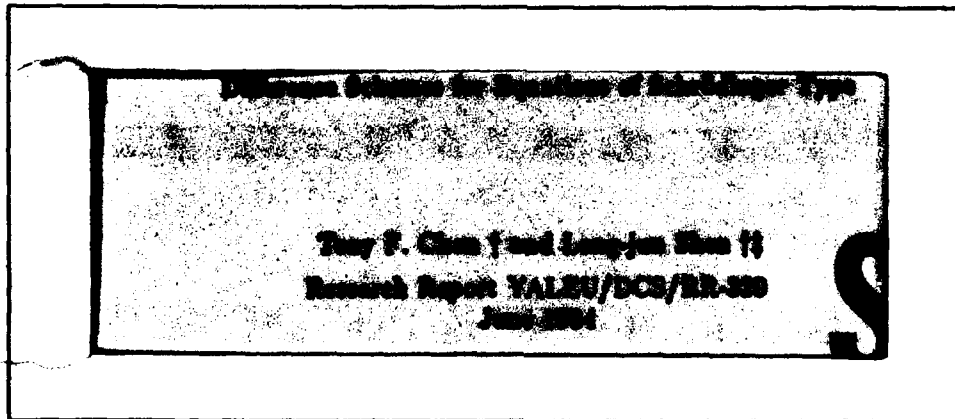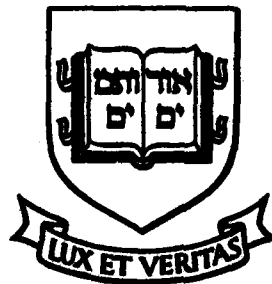UNCLASSIFIED   N00014-82-K-0184   F/G 12/1   NL

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Tony F. Chan † and Langdon White †‡

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We introduce and analyze a collection of difference schemes for the numerical solution of the following equation of Schrödinger type: $u_t = (\alpha + i\beta)u_{xx}$. This includes explicit and implicit schemes, 2-level and 3-level schemes and real and complex schemes. Many of these are analogous to classical schemes for the heat equation and the wave equation but some schemes are unique to the Schrödinger equation. Von Neumann type stability results are given for all the schemes and extensions to higher dimensions are derived in most cases. Many of stability results are quite different from the corresponding results for the heat equation and the wave equation.

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Difference Schemes for Equations of Schrödinger Type

Tony F. Chan † and Long-jun Shen †‡

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1. Introduction

Equations of the Schrödinger type arise in many disciplines, such as quantum mechanics, fluid mechanics, plasma physics, laser propagation, acoustics and optics [4, 5, 19, 23, 25, 27, 34, 35, 36, 37]. This paper is primarily concerned with the numerical solution of the equation

$$u_t = Au_{ss}, \tag{1.1}$$

with $A \equiv a + ib$ and $a \geq 0$, and its extension to higher dimensions:

$$u_t = \sum_{l=1}^{m} A_l u_{s_l s_l} \tag{1.2}$$

where $A_l = a_l + ib_l$, with $a_l \geq 0$ and b_l real, and $a_l^2 + b_l^2 \neq 0$ for $l = 1, \cdots, m$.

Equation (1.1) includes both the heat equation $u_t = au_{ss}$ and the Schrödinger equation $u_t = ibu_{ss}$. It is well known that a rather complete collection of stability results for difference schemes exist for the heat equation [29]:

$$u_t = a\, u_{ss}. \tag{1.3}$$

and for the advection-diffusion equation [6, 9]:

$$u_t = a\, u_{ss} + b\, u_s. \tag{1.4}$$

It is our intention to provide a similar collection of results for the Schrödinger equation. We propose a collection of finite difference schemes, and analyze their accuracy and stability properties. Some of the schemes are analogous to well-known schemes for the wave equation and the heat equation but others are unique to the Schrödinger equation. This includes explicit and implicit schemes, 2-level and 3-level schemes and real and complex schemes. Many of these are analogous to classical schemes for the heat equation but some schemes are unique to the Schrödinger equation. Von Neumann type stability results are derived for all the schemes and extensions to higher dimensions are derived in most cases. Many of stability results are quite different from the corresponding results for the heat equation and the wave equation.

The existence, uniqueness and regularity properties of equations of the Schrödinger type have been investigated in recent years [2, 3, 14, 17, 25, 34, 39]. We are mainly going to discuss finite difference methods for such equations. Among the numerical methods for these equations, the finite difference method is not only a basic one, but also one of the most extensively used. Since many conventional explicit schemes are unconditionally unstable for the Schrödinger's equation [1, 16, 19, 23], implicit schemes have been the most popular — especially the Crank-Nicolson scheme. These results can be found in [1, 10, 11, 15, 16, 19, 23, 27]. Recently, it has been found that stable explicit schemes for equations of the Schrödinger type can be derived if appropriate dissipative terms are added [8] and some of these explicit schemes have been applied to underwater acoustics problems [7]. The articles [16, 40] investigate the existence and convergence of implicit schemes. In recent years, the trend of applying spectral methods [4, 5, 12, 13, 18, 28, 35, 36, 37, 38] and the finite element methods [11, 16, 31] is increasing as well. Methods of lines methods have also been used [22, 24]. Since the solutions of nonlinear equations of the Schrödinger type often possess conservation laws, attempts have also made to construct schemes which satisfy discrete conservation laws. To achieve this, M. Delfour et. al [11] modified the Crank-Nicolson scheme and J.M. Sanz-Serna, and V.S. Manoranjan [30] used the Leap-frog technique. Among three level

schemes, the Leap-frog scheme has been suggested [31]. In [15], predictor-corrector schemes are discussed. For applications of some of the schemes proposed in this paper, the reader is referred to the references [7, 20, 21, 23].

In Sec. 2, our definition of stability is given, as well as a general method for deriving stability results from the characteristic polynomial of a numerical scheme. In Sec. 3, the special case $a = 0$ is considered first and the issue of the existence of stable 2-level explicit schemes is addressed. In Sec. 4, we consider a general two-level scheme for (1.1). In Sec. 5, 6 and 7, we consider 3-level schemes: the Leap-frog scheme, the Du-Fort Frankel scheme and the backward difference scheme. In Sec. 8, we separate the real and imaginary parts of (1.1), and consider schemes that are specifically designed for the resulting system of real equations.

Throughout this paper, k denote the temporal mesh size, h the spatial mesh size, $r \cong \frac{k}{h^2}$, $\eta = 4\sin^2\frac{\theta}{2}$, $0 \le \theta \le 2\pi$ and $\gamma = r\eta$.

2. Definition of Stability and The Schur-Cohn Theory

The usual von Neumann type definition of stability requires that the roots R_j of the characteristic polynomial of a numerical scheme satisfy

$$|R_j| \le 1 + O(k) \tag{2.1}$$

[29]. While this is the appropriate definition of stability for proving convergence as k and h tend to zero, in conjunction with the Lax-Equivalence theorem [29], for practical computations with *fixed* k and h this definition allows the numerical solution to grow with the number of time steps taken. For equations the solutions of which are known to be nonincreasing in time, as is the case for (1.1), this is often undesirable. Hence, for the stability of a numerical scheme, we shall require that the numerical solutions also do not grow in time. This definition of stability is sometimes known as the *practical stability criteria* [29] and is slightly stricter than the definition (2.1). In the absence of lower order terms (e.g. u_s or u) or in the limit as k and h tend to zero, the difference between the two definitions of stability is usually very slight. In what follows, we shall make this definition of stability more precise and outline a procedure for systematically deriving stability conditions for a given numerical scheme.

We shall follow the methodology developed in [6, 9]. We define two classes of polynomials:

Definition 2.1. :
We shall call polynomials $\phi(z)$ with roots R_j *Schur Polynomials* if $|R_j| < 1 \quad \forall j$, and *Simple von Neumann Polynomials* if $|R_j| \le 1 \quad \forall j$ and the roots with magnitude equal to one are distinct.

Let $\phi(z)$ be the characteristic polynomial corresponding to a particular scheme, obtained via Fourier analysis [29].

Definition 2.2. :
A numerical scheme is defined to be *stable* if its characteristic polynomial is Simple von Neumann.

To determine whether a polynomial is a Simple von Neumann polynomial, we shall use the theory of Schur [26, 33, 32]. This theory enables one to determine conditions on the coefficients of the characteristic polynomial for it to be Simple von Neumann.

Given a polynomial

$$\phi(z) = a_0 + a_1 z + \cdots + a_\nu z^\nu \equiv \sum_{j=0}^{\nu} a_j z^j,$$

of degree ν (with $a_\nu \neq 0, a_0 \neq 0$), one can associate with ϕ another polynomial ϕ^*, defined by

$$\phi^*(z) = \sum_{j=0}^{\nu} \tilde{a}_j z^j,$$

where $\tilde{a}$ denotes the complex conjugate of a. The reduced polynomial ϕ_1 is defined by

$$\phi_1(z) = (\phi^*(0)\phi(z) - \phi(0)\phi^*(z))/z.$$

By defintion, the degree of ϕ_1 is one less than that of ϕ. The main results that we need are contained in the following two theorems:

Theorem 2.1. ϕ is a *Schur Polynomial* iff $|\phi^*(0)| > |\phi(0)|$ and ϕ_1 is a *Schur Polynomial*.

Theorem 2.2. ϕ is a *Simple von Neumann Polynomial* iff either (1) $|\phi^*(0)| > |\phi(0)|$ and ϕ_1 is a *Simple von Neumann Polynomial*, or (2) $\phi_1 \equiv 0$ and ϕ' is a *Schur Polynomial* (ϕ' denotes the derivative of ϕ with respect to its dependent variable).

By repeated applications of the above two theorems, it is possible to reduce the question of whether an n-th degree polynomial is a Simple von Neumann Polynomial to that for a first degree polynomial, which can be solved more easily by analytical means. This procedure turns out to be very effective for determining stability limits of general numerical schemes, as compared to first finding the roots of the characteristic polynomial explicitly and then determining conditions for their absolute values to be less than unity. Furthermore, this last approach may not even be applicable for polynomials of higher degrees which arise in the analysis of multi-level schemes and systems of equations (see Sec. 8). Finally, it is worth noting that this reduction process preserves the necessity and sufficiency of the stability conditions.

3. Stable Explicit Schemes for $u_t = iu_{ss}$

We shall first consider the more special equation

$$u_t = iu_{ss}. \tag{3.1}$$

Even in this simple case, the stability properties of some popular schemes are quite different from that for the superficially similar heat equation $u_t = u_{ss}$.

3.1. Taylor Series Schemes

Consider the basic Euler Scheme:

$$\frac{u_j^{n+1} - u_j^n}{k} = iD_j^n u, \tag{3.2}$$

$$\text{where} \qquad D_j^n u \equiv \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}. \tag{3.3}$$

The truncation error is $O(k, h^2)$. The corresponding characteristic polynomial is

$$\phi(z) = z - (1 - i\gamma). \tag{3.4}$$

Since the only root is $R = 1 - i\gamma$ and $|R|^2 = 1 + \gamma^2 > 1$ for $\gamma \neq 0$, $\phi(z)$ is not Simple von Neumann, and thus the Euler scheme is unconditionally unstable, as is well-known [8, 23].

The Euler scheme is the first member of a class of schemes derived from the following Taylor series expansion of a solution $u(x,t)$ of (1.1):

$$u(x, t + k) = u(x, t) + ku_t + \frac{k^2}{2}u_{tt} + \frac{k^3}{6}u_{ttt} + \cdots$$
$$= u(x, t) + k(iu_{xx}) + \frac{k^2}{2}(i^2 u_{xxxx}) + \cdots \tag{3.5}$$

A family of schemes can be derived from (3.6) by replacing the spatial derivatives by difference operators, namely:

$$\frac{u_j^{n+1} - u_j^n}{k} = \sum_{l=1}^{p} \frac{k^{l-1}}{l!} \left(i D_j^n\right)^l u.$$

The truncation error is $O(k^p, h^2)$. The Euler scheme corresponds to $p = 1$. By retaining the next term in the expansion ($p = 2$), we obtain the following Lax-Wendroff type scheme:

$$\frac{u_j^{n+1} - u_j^n}{k} = i D_j^n u - \frac{k}{2}(D_j^n)^2 u.$$

The truncation error is $O(k^2, h^2)$. The corresponding characteristic polynomial is

$$\phi(z) = z - \left(1 - i\gamma - \frac{\gamma^2}{2}\right).$$

Since the only root is $R = \left(1 - \frac{\gamma^2}{2}\right) - i\gamma$ and

$$|R|^2 = \left(1 - \frac{\gamma^2}{2}\right)^2 + \gamma^2 = 1 + \frac{\gamma^4}{4} > 1 \quad \text{for} \quad \gamma \neq 0,$$

this scheme is also unconditionally unstable [8].

Since the first two members of this family of schemes are unconditionally unstable, it is of theoretical interest to determine whether there is any member that is conditionally stable. Moreover, this has practical implications as well, because simple explicit schemes are easier to implement (and vectorize) than implicit schemes, especially for higher dimensional problems.

The third order (in time) scheme derived this way has a characteristic polynomial given by

$$\phi(z) = z - \left(1 - i\gamma - \frac{\gamma^2}{2} + \frac{i\gamma^3}{6}\right).$$

Since

$$|R|^2 = \left(1 - \frac{\gamma^2}{2}\right)^2 + \left(\gamma - \frac{\gamma^3}{6}\right)^2 = 1 - \frac{\gamma^4}{12} + \frac{\gamma^6}{36},$$

the condition that $\phi(z)$ be Simple von Neumann reduces to

$$\max_{\gamma}\left(\frac{\gamma^4}{12} - \frac{\gamma^6}{36}\right) \leq 0,$$

which is satisfied if and only if $\gamma \leq \sqrt{3}$. The stability condition is thus

$$r \leq \frac{\sqrt{3}}{4}.$$

Fot the fourth order scheme, we have

$$\phi(z) = z - \left(1 - i\gamma - \frac{\gamma^2}{2} + \frac{i\gamma^3}{6} + \frac{\gamma^4}{24}\right).$$

After a similar computation, it can be verified that this scheme is stable if and only if $r \leq \frac{\sqrt{3}}{2\sqrt{2}}$.

We thus see that there are stable members in this family of schemes. Unfortunately, while the third and fourth order schemes are conditionally stable, they are not very practical for initial *boundary* value problems because their spatial stencils extends over 7 (resp. 9) points, which makes the construction of stable numerical boundary conditions difficult.

This leads to a natural question:

Does there exist stable explicit schemes with smaller stencils?

3.2. Schemes With Artificial Dissipation

The answer to this question is positive. As shown in [8], stable explicit schemes with a 5-point stencil can be derived from the Euler scheme by adding appropriate dissipative terms. Although the addition of dissipation to stabilize a numerical scheme is rather natural, the question remains as to whether this is the only way to obtain a stable scheme for (3.1). In what follows we shall answer this in the positive by deriving the dissipative schemes in [8] from a general sheme with a 5-point spatial stencil that satisfies certain symmetry conditions.

Suppose an explicit scheme to solve (3.1) takes the form

$$\frac{u_j^{n+1} - u_j^n}{k} = \sum_l c_{j+l} u_{j+l}^n. \tag{3.6}$$

Of course, $\sum_l c_{j+l} u_{j+l}^n$ must be a consistent approximation of $i u_{xx}$ for (3.6) to be consistent with (3.1). Using Taylor expansion, we find that the following consistency conditions must be satisfied:

$$\sum_l c_{j+l} = 0$$
$$\sum_l l c_{j+l} = 0 \tag{3.7}$$
$$\sum_l l^2 c_{j+1} = \frac{2i}{h^2}.$$

If we look for schemes with symmetry, i.e. $c_{j+l} = c_{j-l}$, then (3.7) becomes

$$c_j + 2\sum_{l>0} c_{j+l} = 0,$$
$$2\sum_{l>0} l^2 c_{j+l} = \frac{2i}{h^2}. \tag{3.8}$$

If we take $l = -1, 0, 1$, i.e., using 3 points to approximate iu_{ss}, from (3.8) we find $c_0 = -\frac{2i}{h^2}$, $c_1 = c_{-1} = \frac{i}{h^2}$. This is just the Euler scheme (3.2) and is unconditionally unstable.

Now, let us take $l = -2, -1, 0, 1, 2$, i.e., using 5 points to approximate iu_{ss}. Following the same procedure as above, we can easily find

$$c_0 = 6c_2 - \frac{2i}{h^2},$$

$$c_1 = c_{-1} = \frac{i}{h^2} - 4c_2,$$

where c_2 is a constant to be determined. We want to determine c_2 such that scheme (3.6) is stable.

Writing $c_2 = \frac{c}{h^2}$, where $c = \alpha + i\beta$ with real constants α, β, (3.6) becomes

$$\frac{u_j^{n+1} - u_j^n}{k} = \frac{1}{h^2}\left[(\alpha + i\beta)(u_{j+2}^n + u_{j-2}^n) + (i - 4(\alpha + i\beta))(u_{j+1}^n + u_{j-1}^n)(6(\alpha + i\beta) - 2i)u_j^n\right].$$

$$(3.9)$$

After some rearrangements, scheme (3.9) can be rewritten into another form:

$$\frac{u_j^{n+1} - u_j^n}{k} = i\left(\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}\right) + (\alpha + i\beta)h^2\left(\frac{u_{j+2}^n - 4u_{j+1}^n + 6u_j^n - 4u_{j-1}^n + u_{j-2}^n}{h^4}\right). \quad (3.10)$$

The last term can be viewed as a dissipative term which is added to the unstable scheme

$$\frac{u_j^{n+1} - u_j^n}{k} = i\left(\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}\right),$$

and the truncation error is $O(k, h^2)$. The root of the characteristic polynomial for (3.9) is

$$R = 1 - ir\eta + (\alpha + i\beta)r\eta^2.$$

Thus we have

$$|R|^2 = (1 + \alpha r\eta^2)^2 + (\beta r\eta^2 - r\eta)^2$$
$$= 1 + (r^2 + 2r\alpha)\eta^2 - 2r^2\beta\eta^3 + r^2(\alpha^2 + \beta^2)\eta^4.$$

The condition $|R|^2 \leq 1$ reduces to

$$(r + 2\alpha) - 2r\beta\eta + r(\alpha^2 + \beta^2)\eta^2 \leq 0,$$

from which it follows that the condition on r is

$$r \leq g(\eta) \equiv \frac{-2\alpha}{\alpha^2\eta^2 + (\beta\eta - 1)^2}.$$

For a finite stability interval, we must have $\alpha < 0$. By differentiating $g(\eta)$, it can be verified that $g(\eta)$ cannot achieve its minimum within the interval $0 \leq \eta \leq 4$. Thus the conditions on r reduces to

$$r \leq \min(g(0), g(4)),$$

i.e.

$$r \leq \min\left(-2\alpha, \frac{-2\alpha}{16\alpha^2 + (4\beta - 1)^2}\right). \quad (3.11)$$

To obtain the scheme with the *least* restrictive stability condition, one should make the right hand side of (3.11) as large as possible. Obviously, one should take $\beta = \frac{1}{4}$. Condition (3.11) then reduces to

$$r \leq \min\left(-2\alpha, -\frac{1}{8\alpha}\right).$$

The right hand side achieves its maximum when $-2\alpha = -\frac{1}{8\alpha}$, or $\alpha = -\frac{1}{4}$. Thus we have for the stability condition:

$$r \leq \frac{1}{2}. \tag{3.12}$$

We summarize the results in the following theorem.

Theorem 3.1. *For any real β and $\alpha < 0$, the sheme (3.10) is conditionally stable, the necessary and sufficient condition being (3.11). The least restrictive stability condition is (3.12) and is obtained when $\alpha = -\frac{1}{4}, \beta = \frac{1}{4}$.*

We can also consider a similar dissipative scheme:

$$\frac{u_j^{n+1} - u_j^n}{k} = i\left(\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}\right) + (\alpha + i\beta)k\left(\frac{u_{j+2}^n - 4u_{j+1}^n + 6u_j^n - 4u_{j-1}^n + u_{j-2}^n}{h^4}\right), \tag{3.13}$$

whose dissipative term is different from (3.10). For (3.13), the following theorem has been proved in [8]:

Theorem 3.2. *The scheme (3.13) is stable if and only if $\alpha \leq -\frac{1}{2}$, except for the half line $\left\{\alpha = -\frac{1}{2}, \beta \leq 0\right\}$, and*

$$r \leq \frac{\beta + \sqrt{-\alpha\left(2\alpha^2 + 2\beta^2 + \alpha\right)}}{4\left(\alpha^2 + \beta^2\right)}. \tag{3.14}$$

The least restrictive stability constraint is

$$r \leq \frac{1}{2} \tag{3.15}$$

and is obtained when $\alpha = -\frac{1}{2}, \ \beta = \frac{1}{2}$.

3.3. Stable Dissipative Schemes in Multi-Dimensions

We next consider the multi-dimensional equation:

$$u_t = \sum_{l=1}^{m} i b_l u_{s_l s_l}.$$

We assume that the b_l's have the same sign.

Without loss of generality, we assume $b_l > 0 \quad (l = 1, \cdots, m)$. We consider the natural extension of scheme (3.10):

$$\frac{u_j^{n+1} - u_j^n}{k} = \sum_{l=1}^{m} b_l \left[iD_{j,l}^n u + (\alpha + i\beta)h_l^2 \left(D_{j,l}^n\right)^2 u \right]. \tag{3.16}$$

Here j represents a multi-index $(j_1, \cdots, j_m)$, $D_{j,l}^n$ is the second order centered difference operator with respect to j_l and h_l is the corresponding mesh size.

Theorem 3.3. *Scheme (3.16) is stable if and only if $\alpha < 0$ and*

$$k \leq \min\left(-\frac{2\alpha}{\sum_{l=1}^{m}\frac{b_l}{h_l^2}}, -\frac{\alpha}{\left[\alpha^2 + (\beta - \frac{1}{4})^2\right]\sum_{l=1}^{m}\frac{b_l}{h_l^2}}\right).$$

The least restrictive stability constraint is

$$k \leq \frac{1}{2\sum_{l=1}^{m}\frac{b_l}{h_l^2}}$$

and is obtained when $\alpha = -\frac{1}{4}$ and $\beta = \frac{1}{4}$.

Proof. See Appendix.

4. A General Two-Level Scheme

4.1. The One Dimensional Case:

We now return to the attention of the more general equation (1.1). We consider the following finite difference scheme for (1.1):

$$\frac{u_j^{n+1} - u_j^n}{k} = \frac{\mu A}{h^2}\left(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}\right) + \frac{(1-\mu)A}{h^2}\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right), \qquad (4.1)$$

where μ is a parameter such that $0 \leq \mu \leq 1$. It is easy to see that when $\mu = 0$, (4.1) is the explicit Euler scheme, when $\mu = \frac{1}{2}$, (4.1) reduces to the Crank-Nicolson scheme and when $\mu = 1$, (4.1) is the fully implicit Backward Euler scheme. The truncation error is $O(k, h^2)$ except it is $O(k^2, h^2)$ for the Crank-Nicolson scheme.

Theorem 4.1.

1. *If $\frac{1}{2} \leq \mu \leq 1$, then Scheme (4.1) is unconditionally stable.*

2. *If $0 \leq \mu < \frac{1}{2}$ and $a > 0$, then (4.1) is conditionally stable, the stability condition is*

$$r \leq \frac{a}{2(1 - 2\mu)(a^2 + b^2)}. \qquad (4.2)$$

3. *If $0 \leq \mu < \frac{1}{2}$ and $a = 0$, then (4.1) is unconditionally unstable.*

Proof. The root of the characteristic polynomial for (4.1) is

$$R = \frac{1 - (1-\mu)a\gamma - i(1-\mu)b\gamma}{1 + \mu a\gamma + i\mu b\gamma}.$$

Therefore

$$|R|^2 = \frac{[1 - (1-\mu)a\gamma]^2 + (1-\mu)^2 b^2\gamma^2}{(1 + \mu a\gamma)^2 + \mu^2 b^2\gamma^2}. \qquad (4.3)$$

The condition $|R|^2 \leq 1$ reduces to

$$\frac{1-2\mu}{2}(a^2+b^2)\gamma - a \leq 0. \tag{4.4}$$

If $\frac{1}{2} \leq \mu < 1$, then (4.4) automatically holds; hence Scheme (4.1) is unconditionally stable. If $0 \leq \mu < \frac{1}{2}$, then the condition (4.4) reduces to (4.2). Clearly, if $a = 0$, (4.2) cannot be satisfied for $r > 0$ and hence is unconditionally stable.

∎

Note that when $b = 0$, (4.2) reduces to the well-known stability condition for the heat equation [29].

4.2. The Multi-Dimensional Case:

In this section, we are going to extend the results in Sec. 4.1 to the case of multi-dimensions. We suppose the equation is of the form (1.2) and consider the natural extension of the scheme (4.1) to multi-dimensions:

$$\frac{u_j^{n+1} - u_j^n}{k} = \mu \sum_{l=1}^m A_j D_{j,l}^{n+1} u + (1-\mu) \sum_{l=1}^m A_j D_{j,l}^n u, \tag{4.5}$$

where we have used the same notation as in Sec. 3.3.

As in Sec. 4.1, here μ is a parameter, $0 \leq \mu \leq 1$. Before we state the stability results for this scheme, we need a few definitions.

Definition 4.1. Define an m-dimensional index vector v to be a vector in R^m with components having values of either 0 or 1. Define I_m to be the set of all m-dimensional index vectors except the vector $\{0, 0, \cdots, 0\}^T$.

Theorem 4.2.

1. If $\frac{1}{2} \leq \mu \leq 1$, then Scheme (4.5) is unconditionally stable.

2. If $0 \leq \mu < \frac{1}{2}$, and $a_l > 0$ for $l = 1, \cdots, m$, then (4.5) is conditionally stable, the necessary and sufficient condition is

$$k \leq \frac{1}{2(1-2\mu)} \min_{v \in I_m} \frac{\sum_{l=1}^m \frac{a_l}{h_l^2} v_l}{\left|\sum_{l=1}^m \frac{A_l}{h_l^2} v_l\right|^2}. \tag{4.6}$$

Proof. The root of characteristic polynomial for (4.5) is

$$R = \frac{1 - (1-\mu) \sum_{l=1}^m A_l \gamma_l}{1 + \mu \sum_{l=1}^m A_l \gamma_l}$$

where

$$\gamma_l = 4r_l \sin^2 \frac{\theta_l}{2}, \qquad 0 \leq \theta_l \leq 2\pi,$$

$$r_l = \frac{k}{h_l^2}.$$

We can easily obtain

$$|R|^2 = \frac{\left[1 - (1 - \mu) \sum_{l=1}^{m} a_l \gamma_l\right]^2 + (1 - \mu)^2 \left(\sum_{l=1}^{m} b_l \gamma_l\right)^2}{\left(1 + \mu \sum_{l=1}^{m} a_l \gamma_l\right)^2 + \mu^2 \left(\sum_{l=1}^{m} b_l \gamma_l\right)^2}. \tag{4.7}$$

Then, from the stability condition $|R| \le 1$, we get

$$g(\gamma_1, \cdots, \gamma_m) \equiv -\sum_{l=1}^{m} a_l \gamma_l + (\frac{1}{2} - \mu) \left[\left(\sum_{l=1}^{m} a_l \gamma_l\right)^2 + \left(\sum_{l=1}^{m} b_l \gamma_l\right)^2\right] \le 0. \tag{4.8}$$

It is clear that (4.8) is true if $\frac{1}{2} \le \mu \le 1$, and (4.5) is unconditionally stable in that case. In the case $0 \le \mu < \frac{1}{2}$, it can be verified that $g(\gamma_1, \cdots, \gamma_m)$ reaches its maximum value in the region $D = \{(\gamma_1, \cdots, \gamma_m), \ 0 \le \gamma_l \le 4r_l, \ l = 1, \cdots, m\}$ only at the boundary of D. Clearly, at $(0, \cdots, 0)$, (4.8) always holds. Hence, we obtain (4.6).

∎

Corollary 4.1. *Suppose $0 \le \mu < \frac{1}{2}$.*

1. *If $a_l = 0$ for some l, then (4.5) is unconditionally unstable.*
2. *If all the b_l have the same sign, then the stability condition is*

$$k \le \frac{1}{2(1 - 2\mu)} \frac{\sum_{l=1}^{m} \frac{a_l}{h_l^2}}{\left|\sum_{l=1}^{m} \frac{A_l}{h_l^2}\right|^2}. \tag{4.9}$$

3. *If $b_l = 0$, $1 \le l \le m$, then the stability condition is*

$$k \le \frac{1}{2(1 - 2\mu)} \frac{1}{\sum_{l=1}^{m} \frac{a_l}{h_l^2}}, \tag{4.10}$$

which is a classical result for the heat equation [29].

Proof. To prove the corollary, note first that if $a_l = 0$, then by choosing $v = (0, \cdots, 0, 1, 0, \cdots, 0)$, with the "1" in the l-th position, in (4.6), we have $k \le 0$ and hence the scheme is unconditionally unstable.

Second, if all the b_l have the same sign, the minimum in (4.6) must occur for $v = \{1, 1, \cdots, 1\}^T$ from which (4.9) follows.

Lastly, if $b_l = 0$, $1 \le l \le m$, then (4.10) follows directly from (4.9).

∎

The result (4.6) can be viewed as the extension of the stability result for the multi-dimensional heat equation. It is easy to see that (4.6) is also the extension of (4.2) in Theorem 4.1.

5. The Leap-Frog Scheme

We now consider some three level schemes. First, we study the Leap-Frog Scheme:

$$\frac{u_j^{n+2} - u_j^n}{2k} = \frac{A}{h^2} \left(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}\right). \tag{5.1}$$

The truncation error is $O(k^2, h^2)$.

Theorem 5.1. *Scheme (5.1) is stable if and only if $a = 0$ and $r < \frac{1}{4|b|}$.*

Proof. The characteristic polynomial is

$$\phi(z) = z^2 + 2(a + ib)\gamma z - 1. \tag{5.2}$$

We shall use the Schur theory outlined in Sec. 2 to determine conditions under which $\phi(z)$ is Simple von Neumann. We have

$$\phi^*(z) = -z^2 + 2(a - ib)\gamma z + 1$$

$$\text{and} \qquad \phi_1(z) = 4a\gamma z.$$

Since $|\phi^*(0)| = |\phi(0)|$, $\phi(z)$ can be simple von Neumann only if $\phi_1(z) \equiv 0$, i.e. $a = 0$. Assuming this, for $\phi(z)$ to be simple von Neumann, $\phi'(z) \equiv 2z + 2ib\gamma$ must be Schur, which leads to the condition $r < \frac{1}{4|b|}$.

∎

The stability result for the Leap-Frog scheme can be easily generalized to higher dimensions. Consider the following scheme for (5.1)

$$\frac{u_j^{n+2} - u_j^n}{2k} = \sum_{l=1}^m A_l D_{j,l}^{n+1} u. \tag{5.3}$$

The corresponding characteristic polynomial is

$$\phi(z) = z^2 + 2\left(\sum_{l=1}^m A_l \gamma_l\right) z - 1.$$

By following the same proof as outlined above, it is easy to derive the following stability condition for (5.3)

$$\left|\sum_{l=1}^m b_l \gamma_l\right| < 1. \tag{5.4}$$

From (5.4) it is straightforward to derive the following:

Theorem 5.2. *Scheme (5.3) is stable if and only if*

$$a_l = 0, \quad l = 1, 2, \cdots, m$$

and

$$k \leq \frac{1}{4\max\{B_p, B_N\}},$$

where

$$B_p \equiv \sum_{b_l > 0} \frac{b_l}{h_l^2} \qquad \text{and} \qquad B_N \equiv \sum_{b_l < 0} \frac{|b_l|}{h_l^2}.$$

6. The Du-Fort Frankel Scheme

This is a well-known scheme for the heat equation. With regard to (5.1), using $\frac{1}{2}\left(u_j^{n+2} + u_j^n\right)$ instead of u_j^{n+1}, we obtain the Du-Fort Scheme:

$$\frac{u_j^{n+2} - u_j^n}{2k} = \frac{A}{h^2} DF_j^{n+1} u, \tag{6.1}$$

where $DF_j^{n+1} u \equiv u_{j+1}^{n+1} - u_j^n - u_j^{n+2} + u_{j-1}^{n+1}$. The truncation error is $O\left(k^2, h^2, \left(\frac{k}{k}\right)^2\right)$.

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Theorem 6.1. *Scheme (6.1) is unconditionally stable.*

Proof. The corresponding characteristic polynomial is

$$\phi(z) = (1 + 2Ar)z^2 - (4Ar\cos\theta)z - (1 - 2Ar).$$

We thus have

$$\phi^\circ(z) = -(1 - 2(a - ib)r)z^2 - (4(a - ib)r\cos\theta)z + (1 + 2(a - ib)r),$$

$$\phi_1(z) = 8arz - 8ar\cos\theta,$$

$$|\phi^\circ(0)|^2 = (1 + 2ar)^2 + 4b^2r^2,$$

$$\text{and} \quad |\phi(0)|^2 = (1 - 2ar)^2 + 4b^2r^2.$$

Since $|\phi^\circ(0)| > |\phi(0)|$ and $\phi_1(z)$ is clearly simple von Neumann, this scheme is unconditionally stable.

∎

The extension of (6.1) to multi-dimensions is:

$$\frac{u_j^{n+2} - u_j^n}{2k} = \sum_{l=1}^m A_l\, DF_{j,l}^{n+1} u \tag{6.2}$$

where $DF_{j,l}^n$ is the DuFort-Frankel operator in the x_l-direction. The characteristic polynomial is

$$\phi(z) = \left(1 + 2k\sum_{l=1}^m \frac{A_l}{h_l^2}\right)z^2 - \left(4k\sum_{l=1}^m \frac{A_l}{h_l^2}\cos\theta_l\right)z - \left(1 - 2k\sum_{l=1}^m \frac{A_l}{h_l^2}\right).$$

By following the same proof as in the one dimensional case, with ar replaced by $k\sum_{l=1}^m \frac{a_l}{h_l^2}$ and br by $k\sum_{l=1}^m \frac{b_l}{h_l^2}$, one can easily prove:

Theorem 6.2. *Scheme (6.2) is unconditionally stable.*

7. The Three Level Backward Difference Scheme

This scheme [6, 29] is

$$\frac{3}{2}\left(\frac{u_j^{n+1} - u_j^n}{k}\right) - \frac{1}{2}\left(\frac{u_j^n - u_j^{n-1}}{k}\right) = A\, D_j^{n+1} u, \tag{7.1}$$

and its truncation error is $O(k^2, h^2)$.

Theorem 7.1. *Scheme (7.1) is unconditionally stable.*

Proof. The characteristic polynomial is

$$\phi(z) = \left(\frac{3}{2} + a\gamma + ib\gamma\right)z^2 - 2z + \frac{1}{2},$$

$$\phi^\circ(z) = \frac{1}{2}z^2 - 2z + \left(\frac{3}{2} + a\gamma - ib\gamma\right),$$

$$\text{and} \quad \phi_1(z) = \left[\left(\frac{3}{2} + a\gamma\right)^2 + b^2\gamma^2\right]z - 2(1 + a\gamma - ib\gamma).$$

It can be verified that

$$|\phi^\circ(0)| > |\phi(0)|$$

and therefore for stability, $\phi_1(z)$ must be simple von Neumann, which gives the condition:

$$\left| \frac{2(1 + a\gamma - ib\gamma)}{\left(\frac{3}{2} + a\gamma\right)^2 + b^2\gamma^2} \right| < 1. \tag{7.2}$$

Let $T \equiv \left(\frac{3}{2} + a\gamma\right)^2 + b^2\gamma^2$, then condition (7.2) is equivalent to

$$4\left((1 + a\gamma)^2 + b^2\gamma^2\right) < T^2$$

$$\text{or} \qquad 4\left(T - \frac{5}{4} + a\gamma\right) < T^2$$

$$\text{or} \qquad (T - 2)^2 + 1 + 4a\gamma > 0$$

which is always satisfied since $a \geq 0$. Therefore, this scheme is unconditionally stable.

∎

The extension of (7.1) to multi-dimensions is

$$\frac{3}{2}\left(\frac{u_j^{n+1} - u_j^n}{k}\right) - \frac{1}{2}\left(\frac{u_j^n - u_j^{n-1}}{2k}\right) = \sum_{l=1}^m A_l\, D_{j,l}^{n+1} u. \tag{7.3}$$

The characteristic polynomial is

$$\phi(z) = \left(\frac{3}{2} + \sum_{l=1}^m a_l\gamma_l + i\sum_{l=1}^m b_l\gamma_l\right)z^2 - 2z + \frac{1}{2}.$$

By following the same proof as in the one dimensional case, with $a\gamma$ replaced by $\sum_{l=1}^m a_l\gamma_l$ and $b\gamma$ by $\sum_{l=1}^m b_l\gamma_l$, one can easily prove:

Theorem 7.2. *Scheme (7.3) is unconditionally stable.*

8. Schemes for the Real System

The schemes considered so far are applied directly to the equation (1.1), which is complex-valued in general. But note that if we let $u = v + iw$ (where v and w are real functions), then we can rewrite (3.2) into the following real system:

$$v_t = av_{ss} - bw_{ss}, \tag{8.1}$$

$$w_t = bv_{ss} + aw_{ss}. \tag{8.2}$$

While any scheme for (1.1) has a direct analog for (8.1) and (8.2), this new system opens up more possibilities for constructing numerical schemes because the individual terms of the right hand side of (8.1) and (8.2) can be treated independently of one another by different methods. It is also straightforward to implement these schemes in *real* arithmetic. In the next two sections, we shall consider a few examples of such schemes.

8.1. A Two-Level Real System Scheme

In this section, we shall consider the following 2-level scheme which is similar to, but effectively different from, the Euler scheme for (1.1).

$$\frac{v_j^{n+1} - v_j^n}{k} = \frac{1}{h^2}\left[a\left(v_{j+1}^n - 2v_j^n + v_{j-1}^n\right) - b\left(w_{j+1}^n - 2w_j^n + w_{j-1}^n\right)\right] \tag{8.3}$$

$$\frac{w_j^{n+1} - w_j^n}{k} = \frac{1}{h^2}\left[b\left(v_{j+1}^{n+1} - 2v_j^{n+1} + v_{j-1}^{n+1}\right) + a\left(w_{j+1}^n - 2w_j^n + w_{j-1}^n\right)\right] \tag{8.4}$$

This scheme appears to be semi-implicit, but actually it is explicit for computing because we can compute v_j^{n+1} from (8.3) explicitly, then substituting v_j^{n+1} into (8.4), we can explicitly compute w_j^{n+1}. It is easy to see that the truncation error of (8.3) and (8.4) is $O(k, h^2)$.

Theorem 8.1. *Scheme (8.3) and (8.4) is stable if and only if*

$$r \leq \frac{1}{2(a + |b|)}. \tag{8.5}$$

Proof. The amplification matrix for this scheme is

$$\begin{aligned}
G &= \begin{pmatrix} 1 & 0 \\ b\gamma & 1 \end{pmatrix}^{-1} \begin{pmatrix} 1 - a\gamma & b\gamma \\ 0 & 1 - a\gamma \end{pmatrix} \\
&= \begin{pmatrix} 1 - a\gamma & b\gamma \\ -(1 - a\gamma)b\gamma & 1 - a\gamma - b^2\gamma^2 \end{pmatrix},
\end{aligned}$$

and the characteristic polynomial is

$$\phi(z) = z^2 - z\left(2(1 - a\gamma) - b^2\gamma^2\right) + (1 - a\gamma)^2.$$

It follows that

$$\phi^*(z) = (1 - a\gamma)^2 z^2 - z\left(2(1 - a\gamma) - b^2\gamma^2\right) + 1$$

$$\text{and} \quad \phi_1(z) = z\left(1 - (1 - a\gamma)^4\right) - \left(1 - (1 - a\gamma)^2\right)\left(2(1 - a\gamma) - b^2\gamma^2\right).$$

Since $|\phi^*(0)| > |\phi(0)|$, $\phi_1(z)$ has to be simple von Neumann for the scheme to be stable.

Defining

$$\lambda \equiv \frac{2(1 - a\gamma) - b^2\gamma^2}{1 + (1 - a\gamma)^2},$$

this reduces to the condition

$$-1 \leq \lambda \leq 1.$$

Since λ can be rewritten as

$$\lambda = \frac{1 + (1 - a\gamma)^2 - \left(a^2 + b^2\right)\gamma^2}{1 + (1 - a\gamma)^2},$$

it can be easily seen that the condition $\lambda \leq 1$ is always satisfied. The condition that $-1 \leq \lambda$ reduces to

$$g(\gamma) \equiv -(a\gamma - 2)^2 + b^2\gamma^2,$$

which is equivalent to the condition

$$\gamma|b| \le 2 - a\gamma,$$

and gives the stability limit

$$r \le \frac{1}{2(a + |b|)}.$$

∎

Note that this scheme spans a stencil identical to that for the Euler scheme but the stability condition is quite different. Unlike the Euler scheme, this scheme is conditionally stable even when $a = 0$. This improvement results from the implicit treatment of the v-term in (8.4) and is a direct consequence of separating the original equations into real and imaginary parts.

At first sight, it may appear possible to switch the role of v and w in (8.1) and (8.2) at alternate time steps, similar in spirit to the ADI method, in order to achieve a combined scheme that is second order in time. Unfortunately, it can be verified that this is not true and the resulting alternating scheme is still first order in time.

8.2. The Two-Level Real System Scheme in Multi-Dimensions

The results in the previous section can be extended to higher dimensions. Consider the equation (5.1) which can be written into the following real system

$$v_t = \sum_{l=1}^{m} a_l v_{s_l s_l} - \sum_{l=1}^{m} b_l w_{s_l s_l},$$

$$w_t = \sum_{l=1}^{m} b_l v_{s_l s_l} + \sum_{l=1}^{m} a_l w_{s_l s_l},$$

(8.6)

and the following scheme:

$$\frac{v_j^{n+1} - v_j^n}{k} = \sum_{l=1}^{m} a_l D_{j,l}^n v - \sum_{l=1}^{m} b_l D_{j,l}^n w,$$

$$\frac{w_j^{n+1} - w_j^n}{k} = \sum_{l=1}^{m} b_l D_{j,l}^{n+1} v + \sum_{l=1}^{m} a_l D_{j,l}^n w,$$

(8.7)

The truncation error for (8.7) is again $O(k, h^2)$.

By replacing the terms $a\gamma$ and $b\gamma$ in the previous proof by $\sum_{l=1}^{m} a_l \gamma_l$ and $\sum_{l=1}^{m} b_l \gamma_l$ respectively, the same proof goes through for (8.7) and we obtain the following stability result:

Theorem 8.2. *Scheme (8.7) is stable if and only if*

$$k \le \frac{1}{2\left(\sum_{l=1}^{m} \frac{a_l}{h_l^2} + \left|\sum_{l=1}^{m} \frac{b_l}{h_l^2}\right|\right)}.$$

8.3. A DuFort-Frankel Leap-Frog Scheme for the Real System

Although the real system (8.1) and (8.2) can result in schemes that have superior stability properties than schemes for the complex equation (1.1), deriving such schemes is not at all automatic. In this section, we shall show that a rather natural scheme for the real system (8.1)

and (8.2) actually has worse stability properties than the corresponding schemes for the complex equation (1.1).

We construct a real 3-level scheme for (8.1), (8.2) as follows:

$$\frac{v_j^{n+1} - v_j^{n-1}}{2k} = \frac{a}{h^2}\left(v_{j+1}^n - v_j^{n+1} - v_j^{n-1} + v_{j-1}^n\right) - \frac{b}{h^2}\left(w_{j+1}^n - 2w_j^n + w_{j-1}^n\right), \tag{8.8}$$

$$\frac{w_j^{n+1} - w_j^{n-1}}{2k} = \frac{b}{h^2}\left(v_{j+1}^{n+1} - 2v_j^{n+1} + v_{j-1}^{n+1}\right) + \frac{a}{h^2}\left(w_{j+1}^n - w_j^{n+1} - w_j^{n-1} + w_{j-1}^n\right). \tag{8.9}$$

This is a combination of Du-Fort Frankel Scheme and Leap-frog Scheme. The truncation error is $O(k^2, h^2, \left(\frac{h}{k}\right)^2)$.

Theorem 8.3.

1. *If $a = 0$, then (8.8), (8.9) (the scheme is equivalent to the complex Leap-frog Scheme) is conditionally stable, the stability condition is*

$$r < \frac{1}{4|b|}. \tag{8.10}$$

2. *If $b = 0$, then (8.8) (8.9) (the scheme is equivalent to the Du-Fort Frankel Scheme for the heat equation) is unconditionally stable.*

3. *If $a \neq 0$ and $b \neq 0$, (8.8) (8.9) is unconditionally unstable.*

Proof. The Fourier transform of (8.8),(8.9) can be written in this form:

$$(1 + 2ar)I\tilde{u}^{n+1} = M\tilde{u}^n + (1 - 2ar)I\tilde{u}^{n-1}, \tag{8.11}$$

where

$$\tilde{u} = \begin{pmatrix} \tilde{v} \\ \tilde{w} \end{pmatrix}, \quad M = \begin{pmatrix} a(4r - \gamma) & 2b\gamma \\ -2b\gamma & a(4r - \gamma) \end{pmatrix},$$

I is the identity matrix and $(\tilde{v}, \tilde{w})$ are the Fourier transform of v and w.

It is easy to verify that M is normal and the eigenvalues $\mu_\pm$ of M are:

$$\mu_\pm = a(4r - 2\gamma) \pm i2|b|\gamma. \tag{8.12}$$

Therefore M can be written as $M = X^{-1}\Lambda X$, where $\Lambda = \begin{pmatrix} \mu_+ & 0 \\ 0 & \mu_- \end{pmatrix}$ and X is a unitary matrix.

Multiply from the left of (8.11) by X, we obtain

$$(1 + 2a\gamma)X\tilde{u}^{n+1} = XM\tilde{u}^n + (1 - 2a\gamma)X\tilde{u}^{n-1}. \tag{8.13}$$

Defining

$$s = \begin{pmatrix} y \\ z \end{pmatrix} = X\tilde{u},$$

we have

$$(1 + 2ar)s^{n+1} = XMX^{-1}s^n + (1 - 2ar)s^{n-1}. \tag{8.14}$$

Due to the property of X and the definition of s, the stability of s and $\hat{u}$ are equivalent. So we need only to discuss the stability of s. Since $XMX^{-1} = \Lambda$, we obtain from (8.14):

$$(1 + 2ar)s^{n+1} = \Lambda s^n + (1 - 2ar)s^{n-1} \tag{8.15}$$

i.e.

$$(1 + 2ar)y^{n+1} = \mu_+ y^n + (1 - 2ar)y^{n-1} \tag{8.16}$$

$$(1 + 2ar)z^{n+1} = \mu_- z^n + (1 - 2ar)z^{n-1}. \tag{8.17}$$

Their characteristic polynomials are

$$\phi_\pm(\lambda) = (1 + 2ar)\lambda^2 - \mu_\pm \lambda - (1 - 2ar). \tag{8.18}$$

From this we can easily derive

$$\phi^*(\lambda) = (-1 + 2ar)\lambda^2 - \mu_\mp \lambda + (1 + 2ar),$$

$$\phi_1(\lambda) = [(1 + 2ar)^2 - (1 - 2ar)^2]\lambda - [(1 - 2ar)\mu_\pm + (1 - 2ar)\mu_\mp] = 0, \tag{8.19}$$

and $\quad \phi'(\lambda) = 2(1 + 2ar)\lambda - \mu_\pm.$

In the case $a = 0$, $|\phi^*(0)| = |\phi(0)|$, and $\phi_1(\lambda) \equiv 0$. Therefore stability requires $\phi'(\lambda)$ to be Schur, which reduces to the condition $|b|\gamma < 1$. The stability condition is thus $r < \frac{1}{4|b|}$.

In the case $a > 0$, $|\phi^*(0)| > |\phi(0)|$, so $\phi_1(\lambda)$ must be Simple von Neumann. The only roots of $\phi_1(\lambda)$ are

$$\lambda_\pm = 1 - \frac{\gamma}{2r} \mp i|b|\gamma.$$

Hence

$$|\lambda_\pm|^2 = \left(1 - \frac{\gamma}{2r}\right)^2 + b^2\gamma^2.$$

Clearly, if $b = 0$, then $|\lambda_\pm|^2 \le 1$ because $0 \le \gamma \le 4r$, and (8.8),(8.9) is stable. If $b \ne 0$, $|\lambda_\pm|^2 = 1 + 16b^2r^2 > 1$ when $\gamma = 4r$ and (8.8),(8.9) is unstable.

∎

Therefore, as far as stability properties are concerned, this scheme is similar to the Leap Frog scheme but is inferior to the complex Du-Fort Frankel Scheme, which is unconditionally stable.

9. Summary and Concluding Remarks

In this paper, we have presented a rather exhaustive collection of difference schemes for the Schrödinger's equation (1.1). This includes explicit and implicit schemes, two and three level schemes and schemes with artificial dissipation. It also includes schemes derived from the real system obtained after separating the solution into its real and imaginary parts.

While many of the schemes are adaptations of well-known schemes for the wave equation and the heat equation, the stability properties are often quite different and we have summarized the main results in Table 1.

Scheme	Error	Stability Condition
Taylor Series for $u_t = iu_{ss}$ $$\frac{u_j^{n+1}-u_j^n}{k} = \sum_{l=1}^{p} \frac{k^{l-1}}{l!}\left(iD_j^n\right)^l u$$	$O(k^p, h^2)$	$p=1$: unstable (Euler) $p=2$: unstable (Lax Wendroff) $p=3$: $r \le \frac{\sqrt{3}}{4}$ $p=4$: $r \le \frac{\sqrt{5}}{2\sqrt{2}}$
General 2-level Scheme $$\frac{u_j^{n+1}-u_j^n}{k} = \mu \sum_{l=1}^{m} A_j D_{j,l}^{n+1} u$$ $$+(1-\mu)\sum_{l=1}^{m} A_j D_{j,l}^n u$$	$\mu \ne \frac{1}{2}$: $O(k, h^2)$ $\mu = \frac{1}{2}$: $O(k^2, h^2)$	(i) $0 \le \mu < \frac{1}{2}$ $\quad a_l = 0$ for some l: unstable all b_l have same sign: $k \le \frac{1}{2(1-2\mu)} \frac{\sum_{l=1}^{m}\frac{a_l}{h_l^2}}{\left|\sum_{l=1}^{m}\frac{A_l}{h_l^2}\right|^2}$ all $b_l = 0$: $k \le \frac{1}{2(1-2\mu)}\frac{1}{\sum_{l=1}^{m}\frac{a_l}{h_l^2}}$ (ii) $\frac{1}{2} \le \mu \le 1$: stable
Euler with dissipative term ku_{ssss} ($a=0$) $$\frac{u_j^{n+1}-u_j^n}{k} = ibD_j^n u + (\alpha|b| + i\beta b)k(D_j^n)^2 u$$ Scheme with least restrictive stability $$\frac{u_j^{n+1}-u_j^n}{k} = ibD_j^n u + \left(-\frac{|b|}{2}+\frac{ib}{2}\right)k(D_j^n)^2 u$$	$O(k, h^2)$ $O(k, h^2)$	$(\alpha \le -\frac{1}{2},\ \beta > 0$ or $\alpha < -\frac{1}{2},\ \beta \le 0)$ $r \le \frac{\beta+\sqrt{-\alpha(2\alpha^2+2\beta^2+\alpha)}}{4(\alpha^2+\beta^2)|b|}$ $r \le \frac{1}{2|b|}$
Euler with dissipative term $h^2 u_{ssss}$ ($a_l = 0$) $$\frac{u_j^{n+1}-u_j^n}{k} = \sum_{l=1}^{m} b_l(iD_{j,l}^n u + (\alpha+i\beta)h_l^2\left(D_{j,l}^n\right)^2 u)$$ Scheme with least restrictive stability $$\frac{u_j^{n+1}-u_j^n}{k} = \sum_{l=1}^{m} b_l\left(i\, D_{j,l}^n u + \frac{1}{4}(-1+i)h^2(D_{j,l}^n)^2 u\right)$$	$O(k, h^2)$ $O(k, h^2)$	$\alpha < 0$ and $k \le \min\left(-\frac{2\alpha}{\sum_{l=1}^{m}\frac{b_l}{h_l^2}}, -\frac{\alpha}{[\alpha^2+(\beta-\frac{1}{4})^2]\sum_{l=1}^{m}\frac{b_l}{h_l^2}}\right)$ $k \le \frac{1}{2\sum_{l=1}^{m}\frac{b_l}{h_l^2}}$

Table 1: Summary of Schemes for $u_t = \sum_{l=1}^{m} A_l u_{s_l s_l}$, $A_l = a_l + ib_l, a_l \ge 0, u = v + iw$.

Next, we would like to comment briefly on the effect of lower order terms (such as u_s and u) on the stability results, which arise in many applications. If we adopt the slightly weaker definition of stability (2.1), under which the necessary and sufficient stability conditions given in Table 1 are still sufficient, then it can be shown [29] that, when lower order terms are present, these conditions remain sufficient to insure convergence of the numerical solution in the limit as k and h tend to

Scheme	Error	Stability Condition
Leap-Frog $$\frac{u_j^{n+2}-u_j^{n}}{2k} = \sum_{l=1}^{m} A_l\, D_{j,l}^{n+1} u$$	$O(k^2, h^2)$	all $a_l = 0$ and $$k \le \frac{1}{4\max\{B_p, B_N\}},$$ where $B_p = \sum_{b_l>0} \frac{b_l}{h_l^2}$, $B_N = \sum_{b_l<0} \frac{\lvert b_l\rvert}{h_l^2}$.
Du-fort Frankel $$\frac{u_j^{n+2}-u_j^{n}}{2k} = \sum_{l=1}^{m} A_l\, DF_{j,l}^{n+1} u$$	$O\left(k^2, h^2, \left(\frac{k}{h}\right)^2\right)$	stable
Backward Difference $$\frac{3}{2}\left(\frac{u_j^{n+1}-u_j^{n}}{k}\right) - \frac{1}{2}\left(\frac{u_j^{n}-u_j^{n-1}}{k}\right) = \sum_{l=1}^{m} A_l D_{j,l}^{n+1} u$$	$O(k^2, h^2)$	stable
2-level Real System Scheme $$\frac{v_j^{n+1}-v_j^{n}}{k} = \sum_{l=1}^{m} a_l D_{j,l}^{n} v - \sum_{l=1}^{m} b_l D_{j,l}^{n} w$$ $$\frac{w_j^{n+1}-w_j^{n}}{k} = \sum_{l=1}^{m} b_l D_{j,l}^{n+1} v + \sum_{l=1}^{m} a_l D_{j,l}^{n} w$$	$O(k, h^2)$	$$k \le \frac{1}{2\left(\sum\limits_{l=1}^{m}\frac{a_l}{h_l^2} + \left\lvert\sum\limits_{l=1}^{m}\frac{b_l}{h_l^2}\right\rvert\right)}$$
Du-fort Frankel-Leap Frog Real System Scheme $$\frac{v_j^{n+1}-v_j^{n-1}}{2k} = a DF_j^n v - b D_j^n w$$ $$\frac{w_j^{n+1}-w_j^{n-1}}{2k} = b D_j^{n+1} v + a DF_j^n w$$	$O\left(k^2, h^2, \left(\frac{k}{h}\right)^2\right)$	$a = 0:\ r \le \frac{1}{4\lvert b\rvert}$ $b = 0:$ stable $a \ne 0$ and $b \ne 0:$ unstable

Table 1: Continued

zero (assuming the scheme is consistent). However, for *fixed* k and h, the numerical solution may grow with each time step while the exact solution decays with time. We plan to further investigate the practical stability of these schemes in the presence of lower order terms.

Stability results are important for at least two reasons: to ensure convergence of the numerical solution to the exact solution as k and h tend to zero, and to ensure that the numerical scheme is insensitive to round-off errors for fixed k and h. The choice of a numerical scheme for a particular application depends on more than just the stability property. In practice, accuracy and efficiency are often the controlling factors. The optimal choice can often only be determined empirically with some experimentation.

While we have limited ourselves to second order centered finite difference schemes for the spatial discretization, and have not considered the use of higher order and finite element and spectral methods, the framework used here can be used to derive thses schemes and their corresponding stability results as well.

10. Appendix: Proof of Theorem 3.3

Proof. The amplification factor is given by

$$R = 1 - \sum_{l=1}^{m} b_l r_l \left[i\eta_l - (\alpha + i\beta)\eta_l^2 \right]$$

where

$$r_l = \frac{k}{h_l^2},$$

and

$$\eta_l = 4\sin^2 \frac{\theta_l}{2}.$$

Stability requires

$$|R|^2 = \left[1 + \sum_{l=1}^{m} \alpha b_l r_l \eta_l^2 \right]^2 + \left[\sum_{l=1}^{m} (b_l r_l \eta_l - \beta b_l r_l \eta_l^2) \right]^2 \le 1.$$

i.e.

$$2 \sum_{l=1}^{m} \alpha b_l r_l \eta_l^2 + \alpha^2 \left(\sum_{l=1}^{m} b_l r_l \eta_l^2 \right)^2 + \left[\sum_{l=1}^{m} (b_l r_l \eta_l - \beta b_l r_l \eta_l^2) \right]^2 \le 0.$$

If we define

$$f_l = \frac{b_l}{h_l^2},$$

then this condition can be written as

$$2\alpha \sum_{l=1}^{m} f_l \eta_l^2 + \alpha^2 k \left(\sum_{l=1}^{m} f_l \eta_l^2 \right)^2 + k \left(\sum_{l=1}^{m} f_l \eta_l - \beta \sum_{l=1}^{m} f_l \eta_l^2 \right)^2 \le 0,$$

or

$$k \le G(\eta_1, \cdots, \eta_m) \equiv -\frac{2\alpha \sum_{l=1}^{m} f_l \eta_l^2}{\alpha^2 \left(\sum_{l=1}^{m} f_l \eta_l^2 \right)^2 + \left(\beta \sum_{l=1}^{m} f_l \eta_l^2 - \sum_{l=1}^{m} f_l \eta_l \right)^2}.$$

Let

$$p = (\eta_1, \cdots, \eta_m)$$

and define

$$D = \{ p; \quad 0 \le \eta_l \le 4, \ l = 1, \cdots, m \}$$

$$D_1 = \left\{ p; \quad p \in D \quad \text{and} \quad \sum_{l=1}^{m} f_l \eta_l \le \beta \sum_{l=1}^{m} f_l \eta_l^2 \right\}$$

$$D_2 = \left\{ p; \quad p \in D \quad \text{and} \quad \sum_{l=1}^{m} f_l \eta_l > \beta \sum_{l=1}^{m} f_l \eta_l^2 \right\}.$$

Clearly, $D = D_1 \cup D_2$.

We separate the two cases: $\beta \geq \frac{1}{4}$ and $\beta < \frac{1}{4}$.

Case I. $\beta \geq \frac{1}{4}$

1. In D_1

   Since

   $$\sum f_i \eta_i \leq \beta \sum f_i \eta_i^2 \quad \text{and} \quad 0 \leq \eta_i \leq 4,$$

   we have

   $$0 \leq \beta \sum f_i \eta_i^2 - \sum f_i \eta_i \leq \beta \sum f_i \eta_i^2 - \frac{1}{4} \sum f_i \eta_i^2$$
   $$= \left(\beta - \frac{1}{4}\right) \sum f_i \eta_i^2,$$

   and therefore

   $$G \geq -\frac{2\alpha \sum f_i \eta_i^2}{\alpha^2 \left(\sum f_i \eta_i^2\right)^2 + \left(\beta - \frac{1}{4}\right)^2 \left(\sum f_i \eta_i^2\right)^2}$$
   $$= -\frac{2\alpha}{\left[\alpha^2 + (\beta - \frac{1}{4})^2\right] \sum f_i \eta_i^2}$$
   $$\geq -\frac{\alpha}{8 \left[\alpha^2 + (\beta - \frac{1}{4})^2\right] \sum f_i}.$$

   On the other hand, in the case $\beta \geq \frac{1}{4}$, $(4, \cdots, 4) \in D_1$, and

   $$G(4, \cdots, 4) = -\frac{\alpha}{8 \left[\alpha^2 + (\beta - \frac{1}{4})^2\right] \sum f_i}.$$

   Hence

   $$\inf_{D_1} G(\eta_1, \cdots, \eta_m) = -\frac{\alpha}{8 \left[\alpha^2 + (\beta - \frac{1}{4})^2\right] \sum f_i}. \tag{10.1}$$

2. In D_2

   Since

   $$\sum f_i \eta_i \leq \left(\sum f_i\right)^{\frac{1}{2}} \left(\sum f_i \eta_i^2\right)^{\frac{1}{2}},$$

   we have

   $$0 < \sum f_i \eta_i - \beta \sum f_i \eta_i^2 \leq \left(\sum f_i\right)^{\frac{1}{2}} \left(\sum f_i \eta_i^2\right)^{\frac{1}{2}} - \beta \sum f_i \eta_i^2,$$

   and therefore

   $$G \geq -\frac{2\alpha}{\alpha^2 (\sum f_i \eta_i^2) + \left[(\sum f_i)^{\frac{1}{2}} - \beta (\sum f_i \eta_i^2)^{\frac{1}{2}}\right]^2}.$$

   Letting

   $$w = \left(\sum f_i \eta_i^2\right)^{\frac{1}{2}},$$

   we have

   $$G \geq S(w) \equiv -\frac{2\alpha}{\alpha^2 w^2 + \left[(\sum f_i)^{\frac{1}{2}} - \beta w\right]^2}.$$

It is easy to see
$$\inf_{D_2} w = 0,$$

and if we define
$$w^* = \sup_{D_2} w,$$

then clearly,
$$w^* \leq \tilde{w} \equiv w(4, \cdots, 4) = 4\left(\sum f_l\right)^2.$$

Because of the form of $S(w)$, it achieves its minimum at the end points of the range of w and so
$$G \geq \min(S(0), S(w^*))$$
$$= \min\left(-\frac{2\alpha}{\sum f_l}, S(w^*)\right).$$

Hence
$$\inf_{D_2} G(\eta_1, \cdots, \eta_m) = \min\left(-\frac{2\alpha}{\sum f_l}, S(w^*)\right). \tag{10.2}$$

From (10.1),(10.2), we have
$$k \leq \min\left(-\frac{\alpha}{8\left[\alpha^2 + (\beta - \frac{1}{4})^2\right]\sum f_l}, -\frac{2\alpha}{\sum f_l}, S(w^*)\right).$$

Since
$$S(w^*) > S(\tilde{w}) \equiv -\frac{\alpha}{8\left[\alpha^2 + (\beta - \frac{1}{4})^2\right]\sum f_l},$$

we have the following stability condition when $\beta \geq 4$,
$$k \leq \min\left(-\frac{\alpha}{8\left[\alpha^2 + (\beta - \frac{1}{4})^2\right]\sum f_l}, -\frac{2\alpha}{\sum f_l}\right). \tag{10.3}$$

Case II. $\beta < \frac{1}{4}$

Clearly, D_1 is empty and $D = D_2$. It is easy to see that
$$G \geq \min\left(S(0), S\left(4\left(\sum f_l\right)^{\frac{1}{2}}\right)\right)$$
$$= \min\left(-\frac{2\alpha}{\sum f_l}, -\frac{\alpha}{\left[\alpha^2 + (\beta - \frac{1}{4})^2\right]\sum f_l}\right).$$

The general stability condition is therefore (10.3). Clearly, we must have $\alpha < 0$. To choose α and β such that the stability condition is the least restrictive, we should take $\beta = \frac{1}{4}$ so that we have
$$k \leq \min\left(-\frac{1}{8\alpha\sum f_l}, -\frac{2\alpha}{\sum f_l}\right).$$

To maximize the right hand side, we should take
$$\alpha = -\frac{1}{4}$$

and the stability condition becomes

$$k \leq \frac{1}{2\sum f_i} \equiv \frac{1}{2\sum \frac{b_i}{h_i^2}}.$$

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